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Asymmetric thermal vibrations of atoms and pyroelectricity in cancrinite

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Abstract

The crystal structure of CO3-cancrinite was analyzed by applying a generalized structure factor expression of the Gram-Charlier expansion to the least-squares refinement performed by using the X-ray intensities measured on single crystals at 173, 293, 473, and 673 K. No satellite reflection or diffuse scattering was observed. The space group is P63 with unit cell a = 1.2604(3) and c = 0.51144(8) nm at 173 K, and a = 1.2709(4) and c = 0.5202(6) nm at 823 K. The temperature behavior for the dehydration and the unit cell dimensions were considerably different from those previously reported for CO3-cancrinite, which shows superstructure reflections.Two position vectors were assigned to each of the framework atom sites or the CO3 site for examining its asymmetric probability density function-one for the free energy minimum and another for the potential energy minimum. Two polarization vectors were obtained for a unit cell from those position vectors and ion charges. The rigid ion contributions to the pyroelectric coefficients p(σ) (measured under a constant stress σ) and the secondary coefficient p(2) were finally estimated from the temperature dependences of the polarization vectors.

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Keywords

Asymmetric thermal vibrations, Cancrinite, Pyroelectricity, Spontaneous polarization